Modeling of Fuzz Formation on Helium-Ion-Irradiated Tungsten Surfaces

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59th Annual Meeting of the APS Division of Plasma Physics, Milwaukee, WI
October 26, 2017

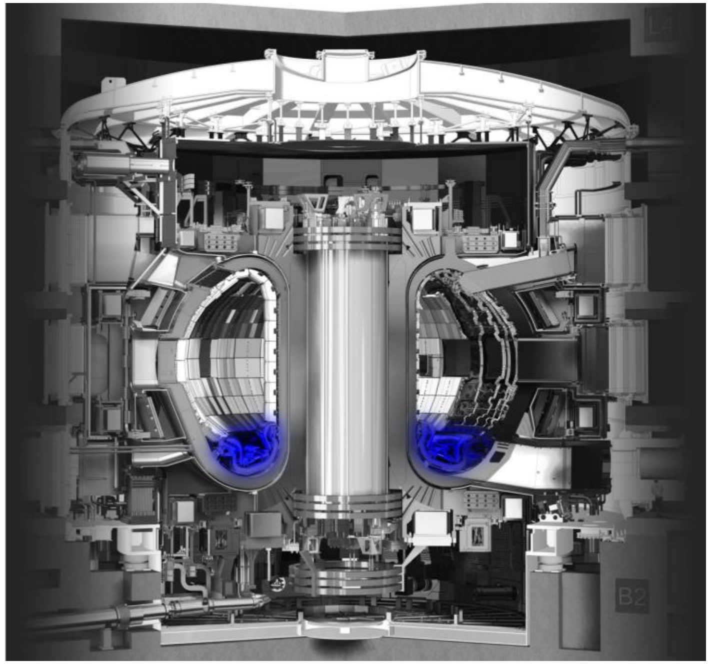
Financial Support:

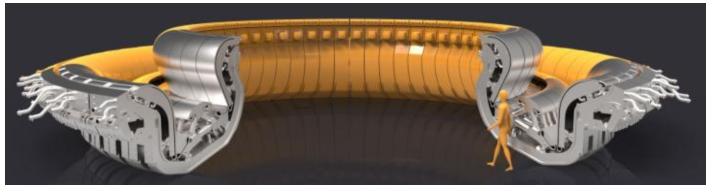
This work was supported by the DOE-OFES and SciDAC through Advanced Computing project on Plasma-Surface Interactions under Award No. DE-SC0008875, and partially supported by OFES Award DE-SC0006661.

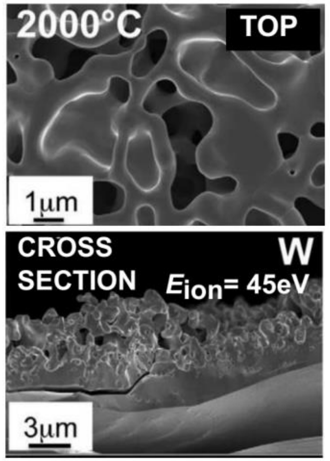
The experimental work was supported by the DOE-OFES, through the Materials and Fusion Nuclear Science and Early Career Research programs.

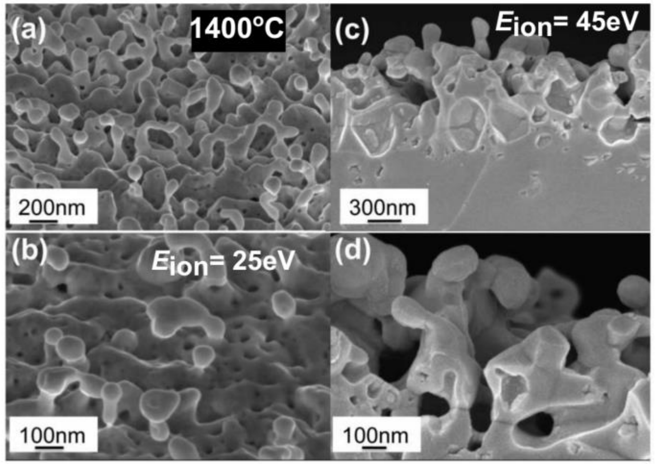
Motivation: Fusion Materials

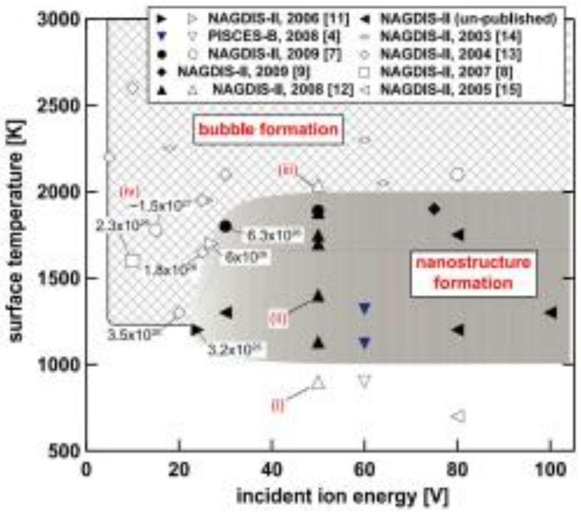
- Plasma facing materials (PFMs): Tungsten
  - Low hydrogen solubility, low sputtering yield, high melting point, and high thermal conductivity
  - He irradiation modifies near surface microstructure: Increase in retention of tritium, fuzz-like nanostructure
  - Divertor of ITER: Nucleation of bubbles, retention of hydrogen isotopes, and production of high-Z dust
- ‘Fuzz’: Temperature (1000-2300K), He energy (~10eV), and He flux





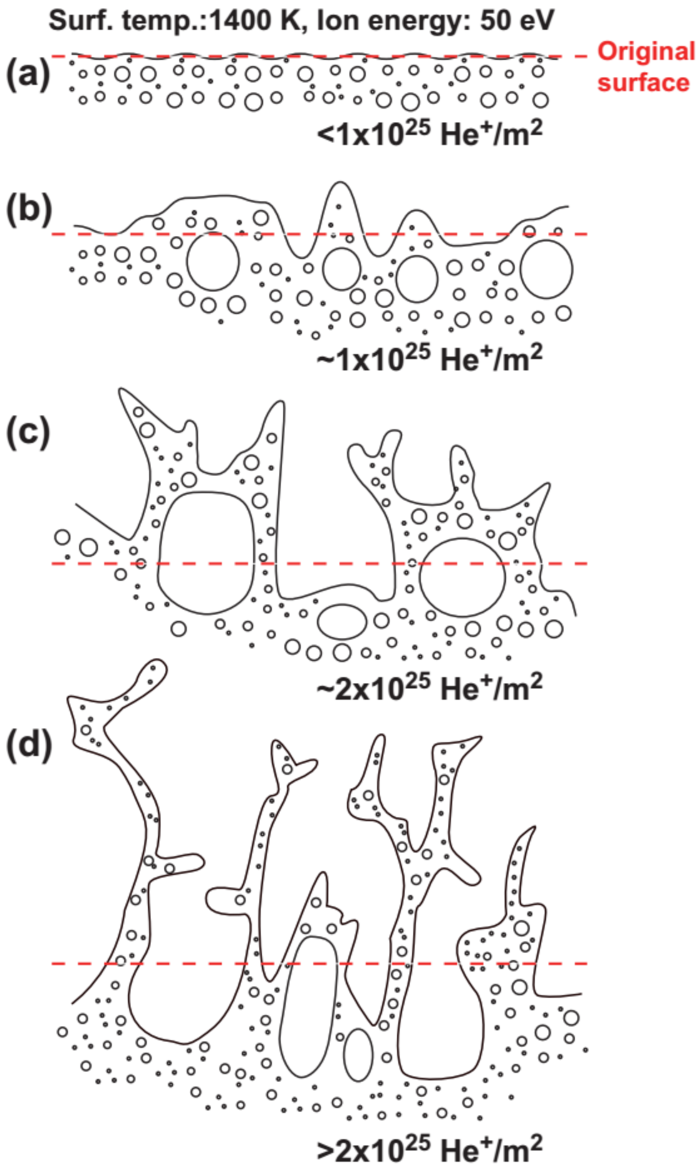






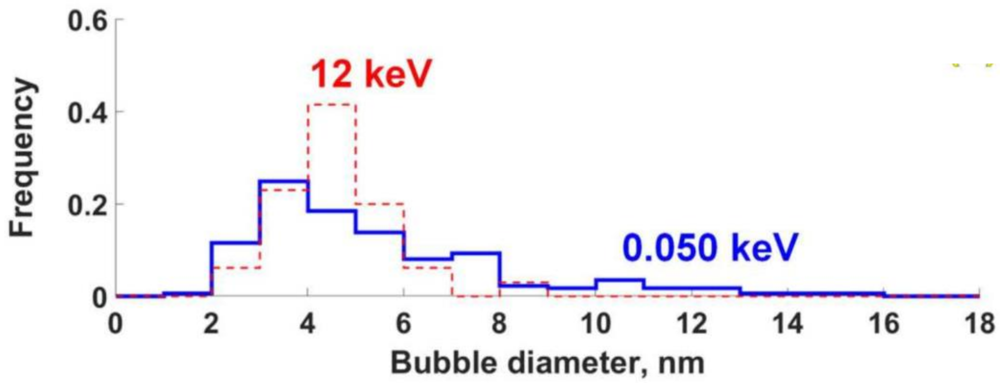
Ref: G. De Temmerman *et al*., J. Vac. Sci. Technol. A 30, 041306 (2012); S. Kajita *et al*., Nucl. Fusion 49, 095005 (2009).

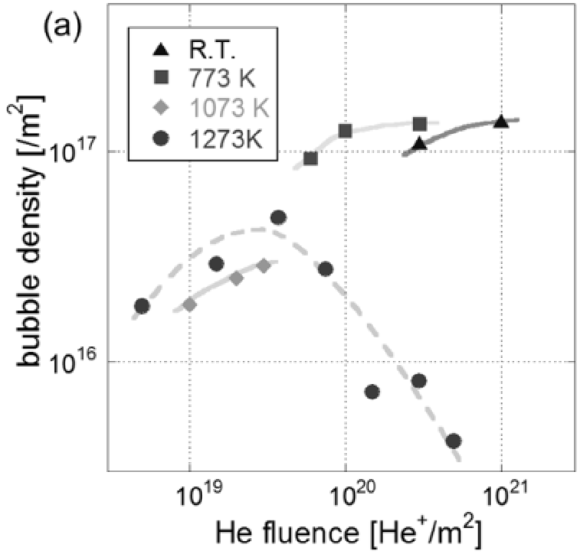
State of Knowledge in the Field



Ref: S. Kajita *et al*., Journal of Nuclear Materials **418**, 152–158 (2011).

- Bubble density in nanobubble layer and bubble diameter depend on the surface temperature and fluence
- The bubbles grow via trap mutation reaction. Bubbles are favorable to grow for bubble concentration $\sim 10^{-40}$/ W
- Surface diffusion, loop punching, and bubble bursting leads to pinholes, dips, and protrusion formation on the surface
- Subsurface bubble growth further propagates the surface morphological evolution; the edge becomes sharper and the dip becomes deeper in this process.

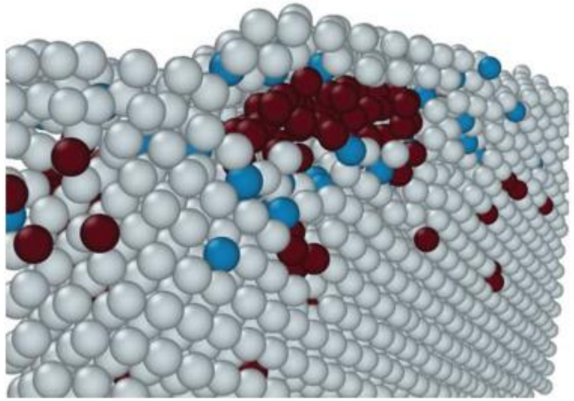


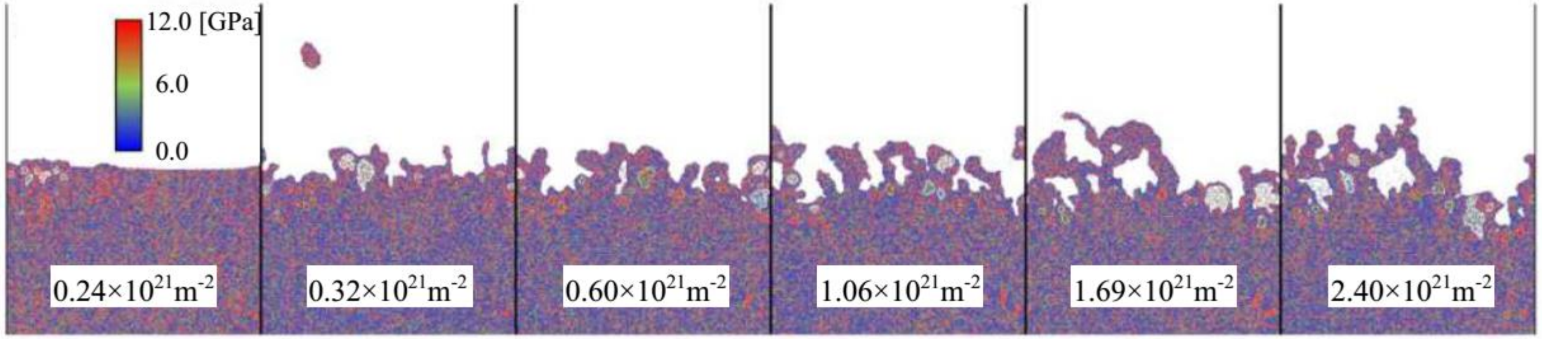


Ref: K. Wang *et al*., Sci. Rep. **7**, 42315 (2017); M Miyamoto *et al*., Phys. Scr. **T159**, 014028 (2014).

State of Knowledge in the Field

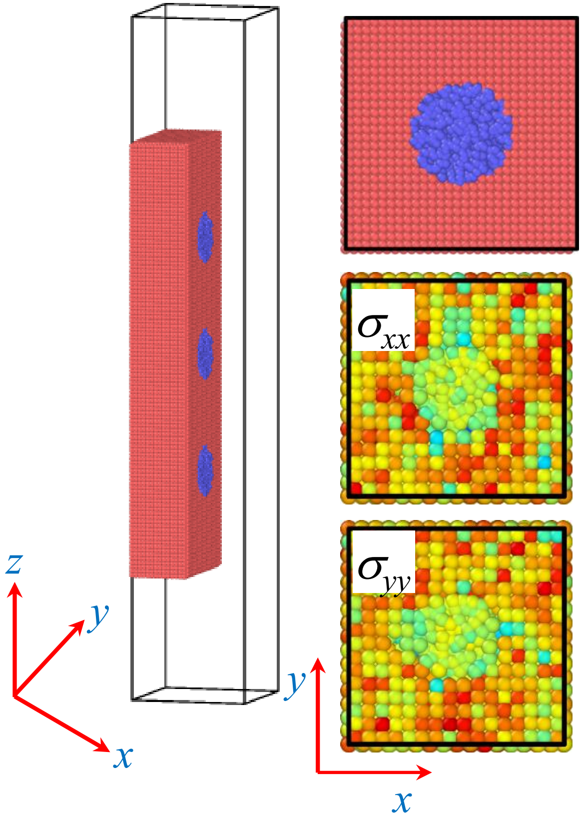
- Viscoelastic model: Viscoelastic W flow from below bubble layer drives fuzz growth. [S. I. Krasheninnikov, Phys. Scr. T145, 014040 (2011).]
- Large scale MD simulations: Successfully predicted subsurface He bubble dynamics but maximum timescale captured so far is $O(10^3\text{ns})$ while onset of fuzz-formation happens $O(10^3\text{s})$. For a typical MD run time on ANL Mira ($O(2 \times 10^7$ atoms) simulation on $O(2 \times 10^4)$ cores), to reach onset of fuzz formation requires $O(300$ Million years) wallclock time. [K. D. Hammond *et al*., Fusion Sci. Technol. 71(1), 7-21 (2017).]
- KMC simulations†: KMC extended the MD results from ns-Å to s-μm scale, but unable to reach the experimental hr-mm range.
- MD and MC hybrid simulations: Semi-2D MD and MC hybrid simulations have captured the fuzz formation.

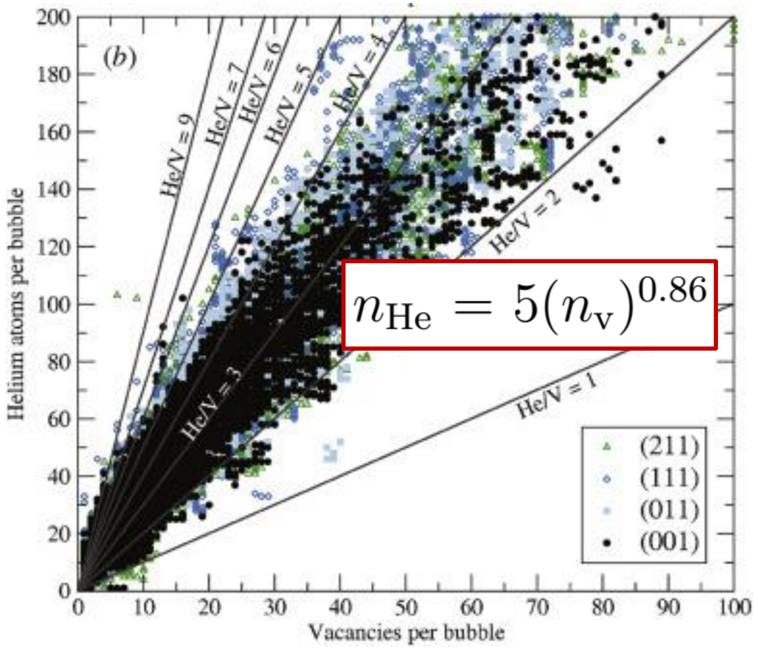


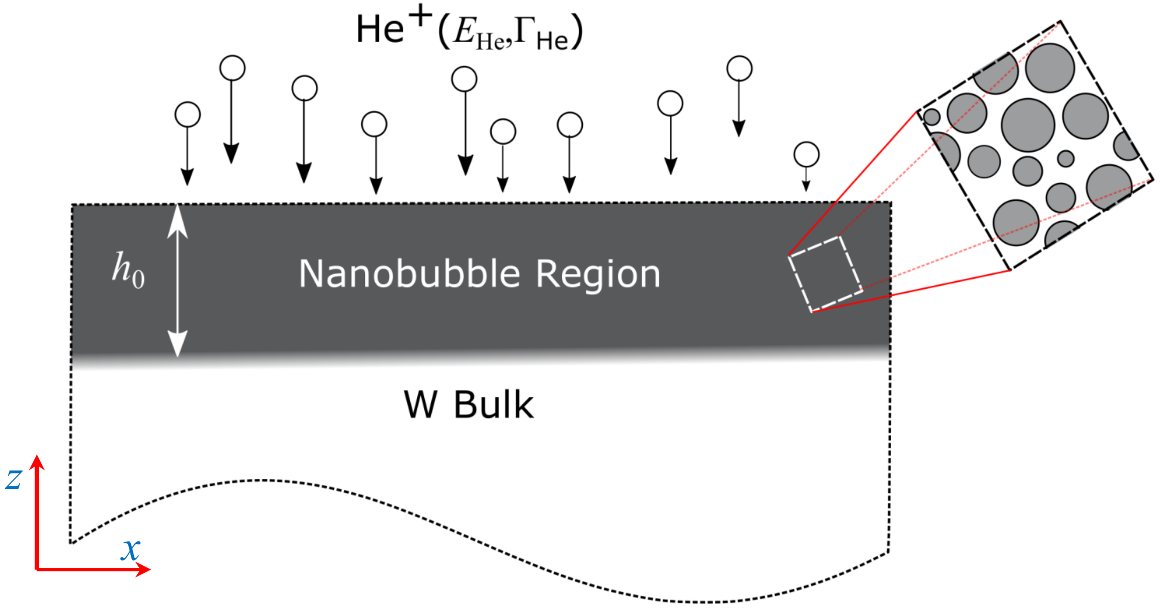


†A. Lasa *et al*., Europhys. Lett. 105, 25002 (2014); A. M. Ito *et al*., Nucl. Fusion 55, 073013 (2015).

Model







- Continuum domain model is based on following assumptions:
  - Nanobubble region is a homogeneous layer of spherical bubbles with uniform size and number density;
  - Nanobubble region is under constant stress due to overpressurized bubble;
  - Subsurface bubble dynamics is not included in the current model.
- Model parameterization relies on material and thermophysical properties obtained through either atomic-scale simulations or experimental results available in the literature [Ref: K. D. Hammond *et al*., Acta Materialia (Article in press); S. E. Donnelly, Radiat. Eff. 90, 1-47(1985)]

Model

- Continuity equation:

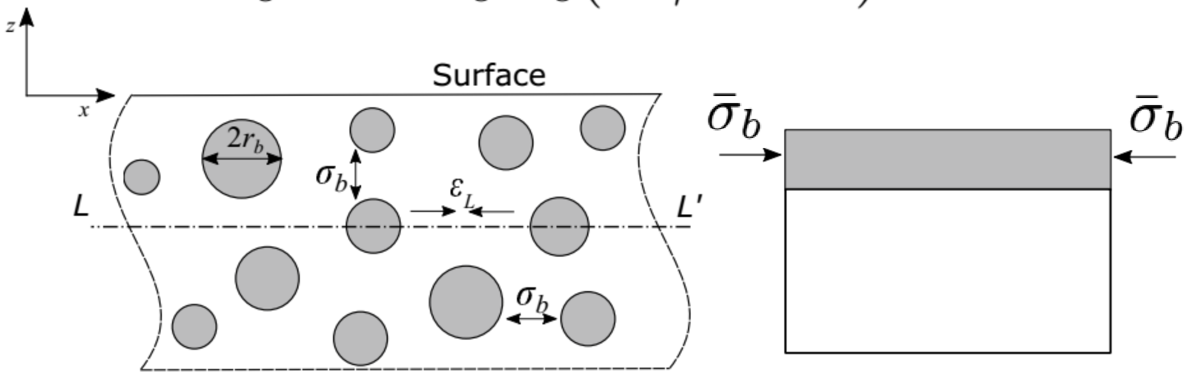
$$\partial_t h = \frac{H'\delta_s}{k_B T}\nabla_s \cdot \mathbf{J}_s + \Omega J_\mathrm{I} - \Omega J_\mathrm{sp}$$

- Sputtering loss (J_sp): $J_\mathrm{sp} = \Gamma_\mathrm{He} Y_\mathrm{sp}$

$$Y_\mathrm{sp} = Y_\infty \left[1 - d_E \left(\frac{\beta}{\alpha}\right)^2 \kappa\right]$$

- Surface mass flux ($\mathbf{J}_s$):

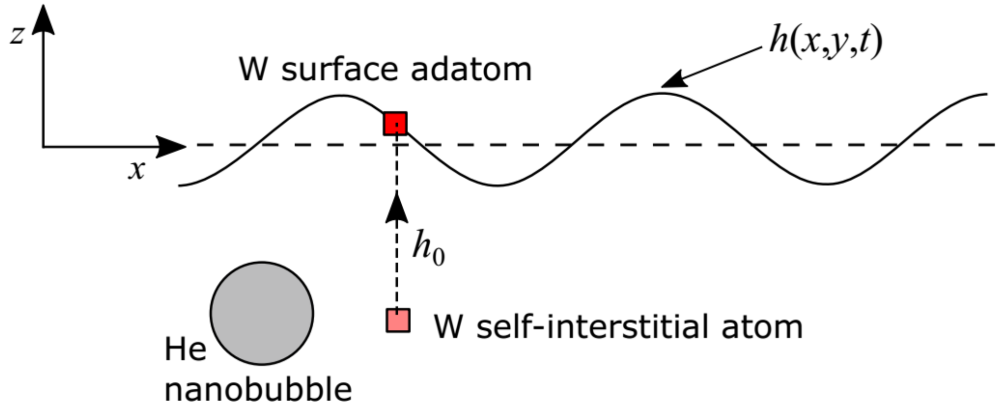
$$\mathbf{J}_s = \Omega D_s \nabla_s(-\gamma\kappa + \mathcal{E})$$



  - Young-Laplace equation for overpressurized bubble
  - Average microscopic stress:

$$\bar{\sigma}_b = \left(p - \frac{2\gamma'}{r_b}\right)\frac{A_b}{1 - A_b}$$

- Interstitial mass flux (J_I):



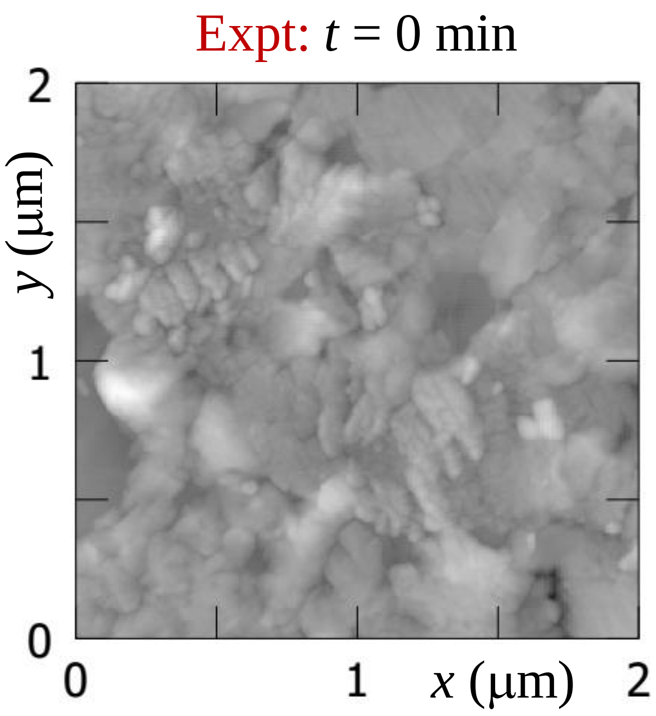
  - Thermodynamic driving force:

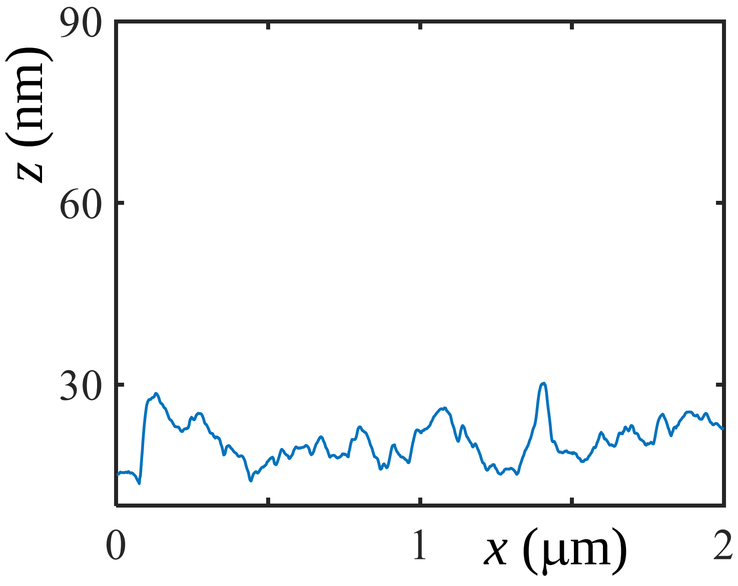
$$-\nabla_z \mu' = -\frac{\Delta\mu'}{\Delta z} = -\frac{\mu - \mu_\mathrm{I}}{0 - (-l_D)}$$

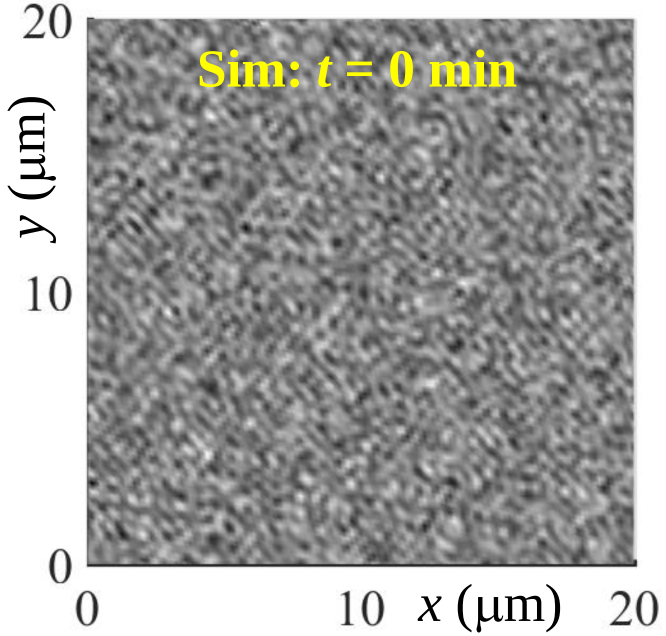
  - Mass-flux:

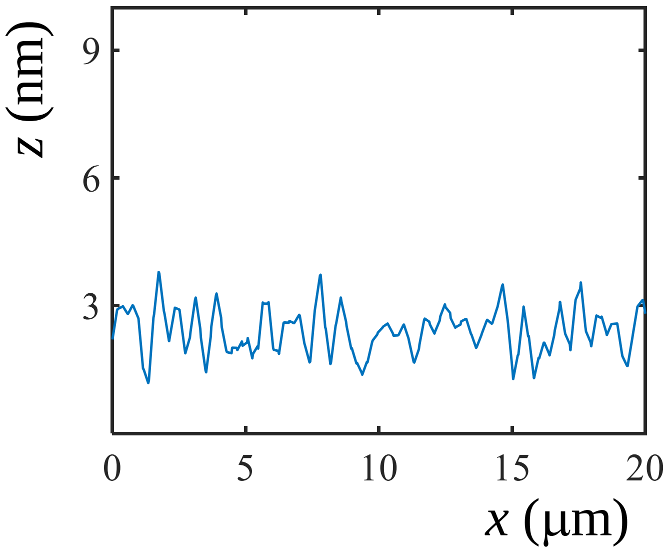
$$J_\mathrm{I} = \frac{D_\mathrm{I} C_{\mathrm{I},0}}{k_B T h_0}\left[\Omega\gamma\kappa - \Omega\mathcal{E}\right] + \mathrm{const.}$$

Results: Benchmarked against Experiments



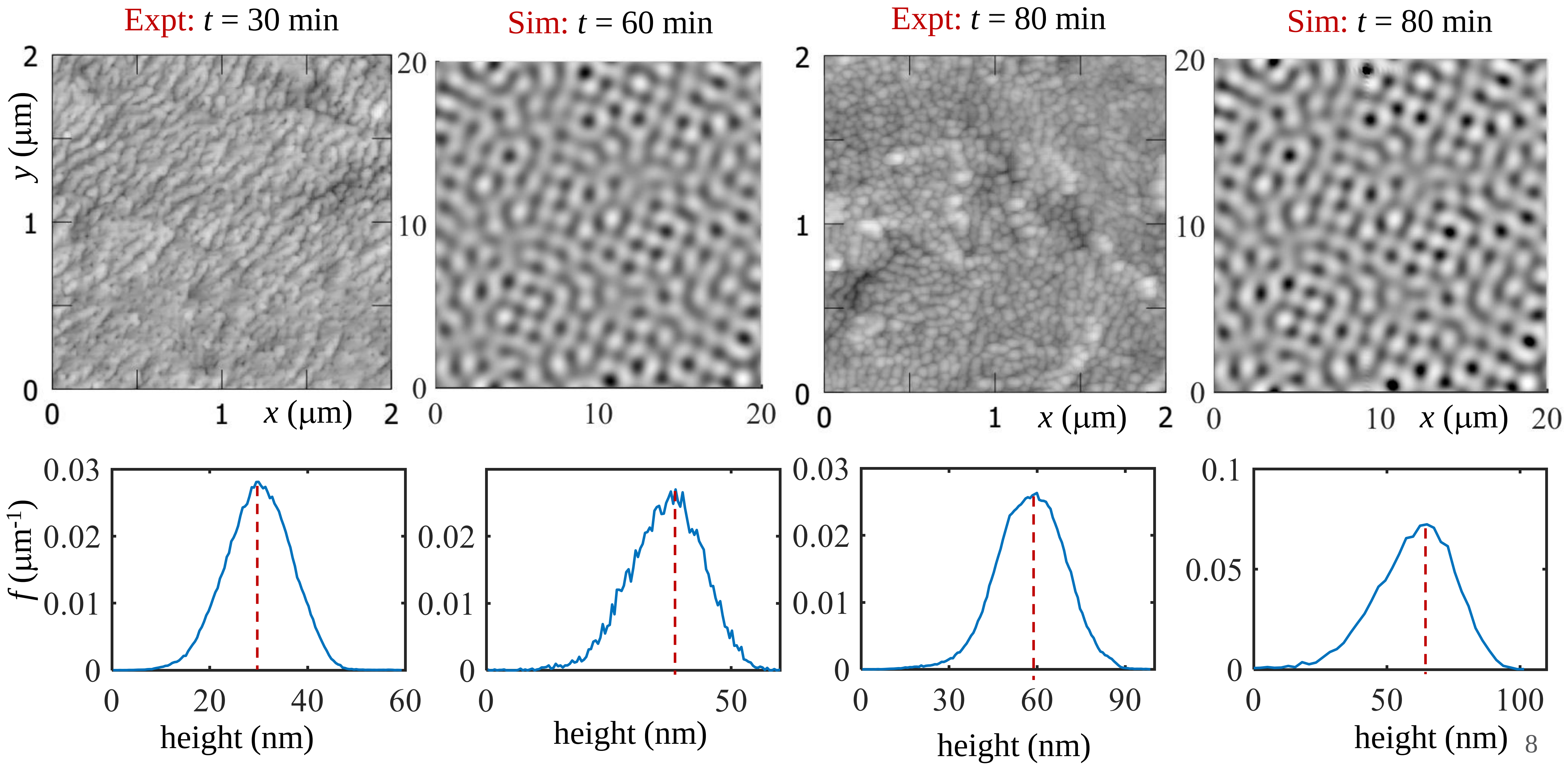




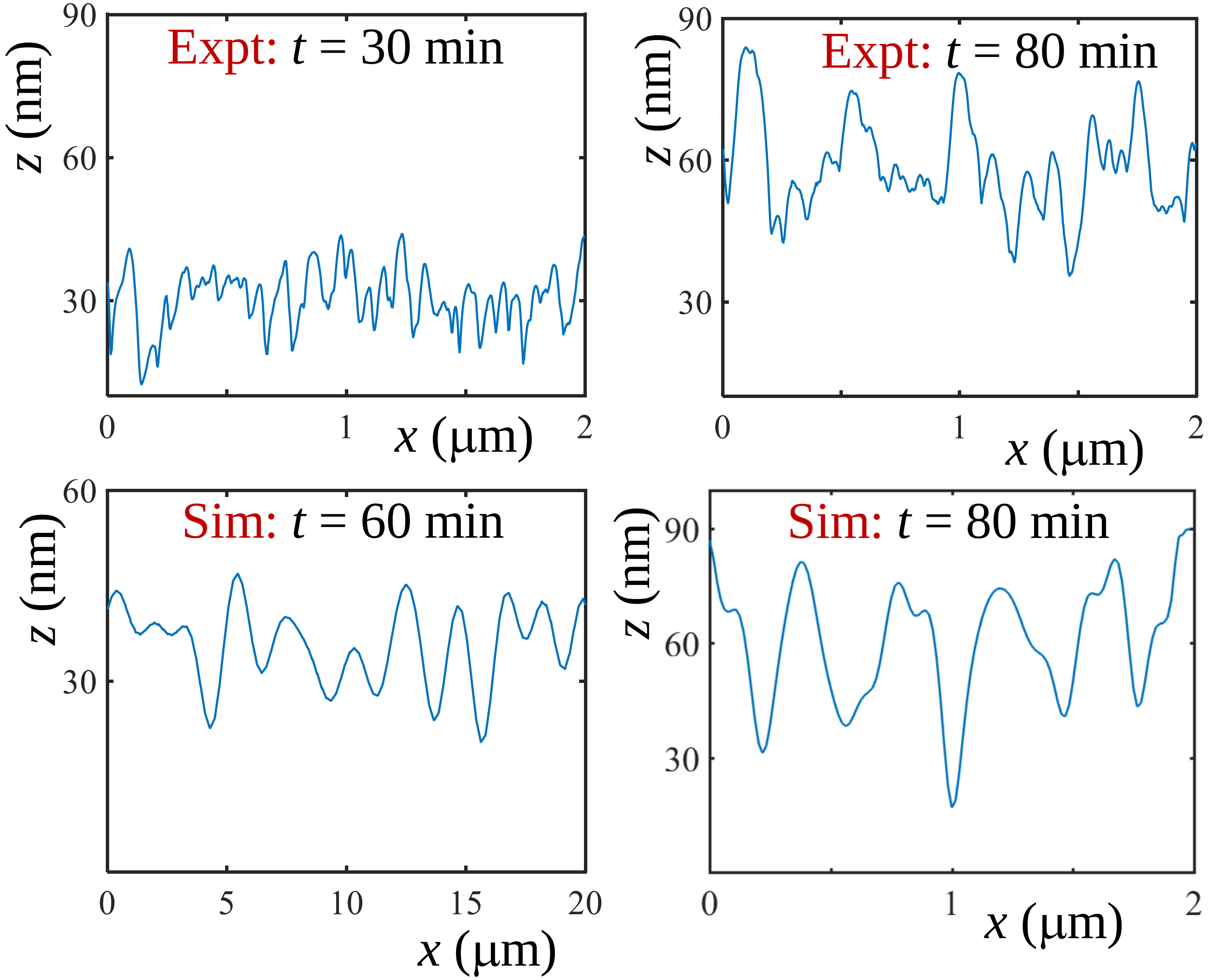


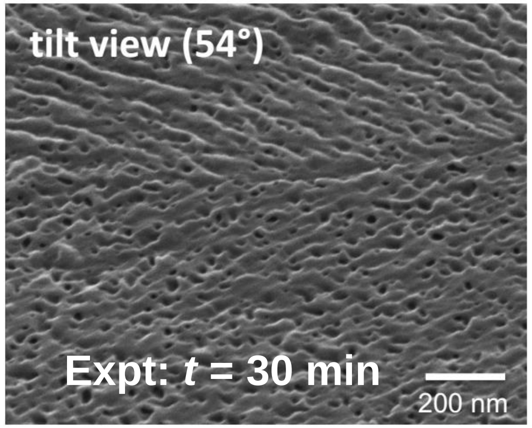
- **Experiment:** A medium-flux RF plasma source (2.7×10^{20} He m^{-2} s^{-1}) was used to expose ITER-grade W specimens to ion fluences ranging between 5×10^{23} – 1.2×10^{25} He m^{-2} (corresponding to exposure times ranging between 30 min. to 12 hrs.). For each test, the sample temperature (840 °C) and incident ion energy (75 eV) were identical
- **Simulation:** The W surface morphology was perturbed with small amplitude normal wave random perturbations (with an rms value, 10^{-4}, much lower than polished W surface). The sample temperature and incident ion energy were identical with experiments. Helium retention was assumed to be ~1%

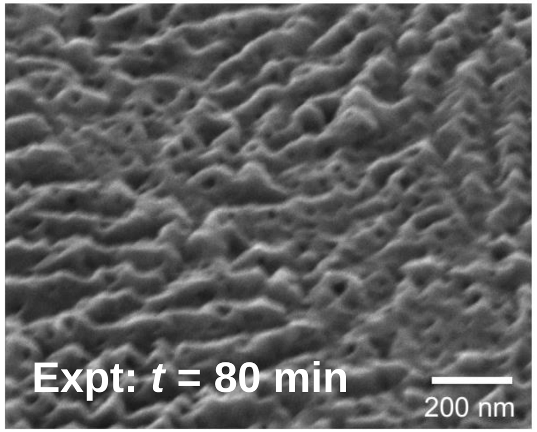
Results: Benchmarked against Experiments

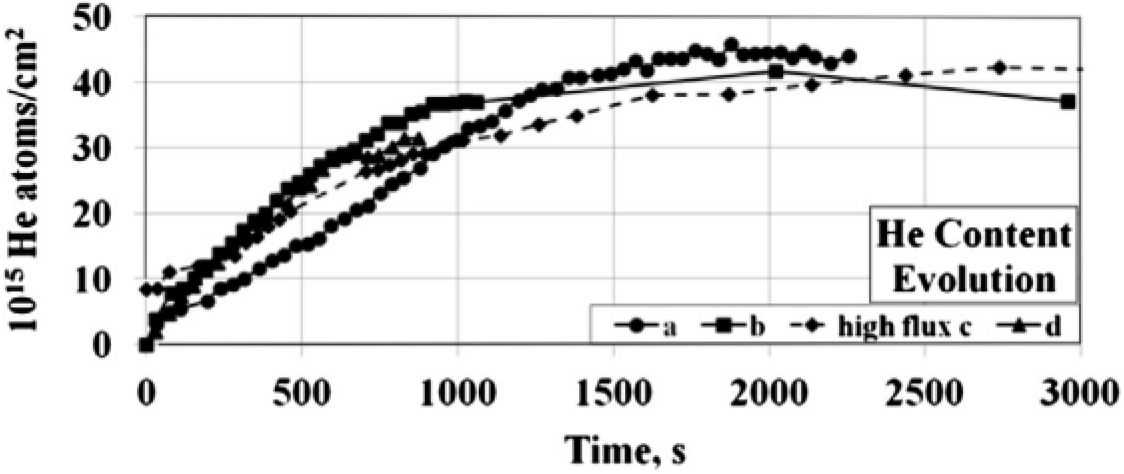


Results: Benchmarked against Experiments









Ref: K.B. Woller *et al.*, J of Nucl. Mater **463**, 289–293 (2015).

- Helium concentration reaches saturation level with negative exponential growth (approximately in 1500 s)
- Bubble bursting/pinhole formation appears to play an important in surface morphological evolution

Summary & Future Work

- An atomistically-informed, continuous-domain model is developed to describe the initial stages of surface deformation, leading to fuzz formation in helium-ion-irradiated tungsten and the simulation results are benchmarked against experimental studies
- A spectral collocation method and discrete fast Fourier transforms are used to compute spatial profile of the field-variables (curvature, stress, etc.). For time stepping, an operator splitting-based semi-implicit spectral method with adaptive time step size is used to carry out self-consistent dynamical simulations. For a typical simulation run time on HPC ($O(1\mu\mathrm{m} \times 1\mu\mathrm{m}$ surface) simulation on single core), to reach onset of fuzz formation requires $O(10$ hours) wallclock time
- Continuum domain model can qualitatively capture nanotendril formation at high temperature; the model predicts the growth rate of nanotendrils reasonably well and nanotendril widths are quantitatively comparable ($\sim$200 nm) with those observed in experimental studies
- Subsurface bubble dynamics and bubble bursting, redeposition of sputtered W, etc. soon to be included in the model
- Model will be benchmarked against measurements from carefully designed experiments at different temperature and gas implantation conditions